

# Monte Carlo study of dynamic phase transition in Ising metamagnet driven by oscillating magnetic field

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The dynamical responses of Ising metamagnet (layered antiferromagnet) in the presence of a sinusoidally oscillating magnetic field are studied by Monte Carlo simulation. The time average staggered magnetization plays the role of dynamic order parameter. A dynamical phase transition was observed and a phase diagram was plotted in the plane formed by field amplitude and temperature. The dynamical phase boundary is observed to shrink inward as the relative antiferromagnetic strength decreases. The results are compared with that obtained from pure ferromagnetic system. The shape of dynamic phase boundary observed to be qualitatively similar to that obtained from previous meanfield calculations.

**Keywords:** Ising metamagnet, Monte Carlo Simulation, Dynamic phase transition.

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## I. Introduction:

The dynamic phase transition[1], in pure Ising ferromagnet driven by oscillating magnetic field, became an interesting field of modern research in nonequilibrium statistical physics. The researchers paid much attention in last few years to study the dynamical phase transition in other magnetic models also. The dynamic transition is studied[2] in kinetic spin-3/2 Blume-Capel model. The multicritical behaviour was observed[3] in kinetic Blume-Emery-Griffith model. The dynamic transition was investigated in the classical Heisenberg model[4] with bilinear exchange anisotropy and in XY model[5]. The multiple dynamic phase transition was also observed[6] in classical anisotropic Heisenberg ferromagnet driven by polarised magnetic field. The existence of dynamic phase transition was found by few experimental studies in systems like ultrathin Co film on Cu(100)[7, 8] by surface magneto-optic Kerr effect.

However all these studies mentioned above are done in simple ferromagnetic systems. Due to the presence of complicated exchange interactions, the dynamical responses of metamagnets driven by oscillating magnetic field may give rise to some interesting effects. Keeping this in mind, recently few researchers have taken interest to study the dynamical behaviours of metamagnets driven by oscillating magnetic field. Few investigations are made in this front. Dynamic phase transition is studied in kinetic metamagnetic[9] spin-3/2 Blume-Capel model, in Ising metamagnets[10] etc. However, all these studies are mainly based on meanfield theory.

In the meanfield calculations the spin fluctuations are ignored and the results do not have any informations of microscopic details. Moreover, the transition is studied only from the temperature variations of the order parameters. The temperature variations of quantity like specific heat cannot be studied. One possible way to incorporate, the fluctuations as well as the temperature variations of specific heat, is to study this by Monte Carlo simulations. As far as the author's knowledge is concerned, no such attempt has been made so far to study the dynamic phase transition, even in simple Ising metamagnet driven by oscillating magnetic field, by Monte Carlo simulation. Being motivated by these facts, the dynamic response of Ising metamagnet driven by oscillating magnetic field, is studied by Monte Carlo simulation, in this article.

The paper is organised in the following manner. The Ising metamagnetic model and the Monte Carlo simulation scheme are discussed in the next

section (section-II). The numerical results are given in section-III. The paper ends with concluding remarks and summary in section-IV.

## II. Model and Simulation:

The time dependent Hamiltonian (or energy) of a three dimensional Ising metamagnet (layered antiferromagnet) is represented as:

$$H(t) = -J_F \sum_F s_i s_j - J_A \sum_A s_i s_j - h(t) \sum s_i. \quad (1)$$

First term represents the in-plane ferromagnetic ( $J_F > 0$ ) nearest neighbour spin-spin interaction energy. Second term provides the interaction energy coming from the antiferromagnetic ( $J_A < 0$ ) interaction between two adjacent layers (since the nearest neighbour interactions are considered only). Third term gives the spin ( $s_i = \pm 1$ )-field ( $h(t)$ ) interaction energy. Here the time dependent field is taken in the sinusoidal form, i.e.,  $h(t) = h_0 \cos(\omega t)$ . The boundary condition is taken periodic in all directions.

A cubic lattice of linear size  $L = 20$  is considered. The dynamical evolution of the Ising spins are studied by Monte Carlo simulation using Metropolis[11] single spin-flip scheme. The initial state of spin configuration is prepared by taking 50 percent of total number of spins (randomly selected) up ( $s_i = +1$ ). This corresponds to a high temperature paramagnetic phase. According to Metropolis[11] single spin flip dynamics, a spin, selected randomly, will flip ( $s_i \rightarrow -s_i$ ) with probability,

$$W(s_i \rightarrow -s_i) = \text{Min}[1, \exp(-\Delta H/K_B T)] \quad (2)$$

where,  $\Delta H$  is the change in energy due to spin flip,  $K_B$  is Boltzmann constant and  $T$  is the temperature.  $L^3$  number of such random updates of spins is one Monte Carlo Step (MCS) and defines the unit of time in the present study. After a long time a dynamical steady state is achieved. The satisfactory steady values of the time averages of the dynamical physical quantities (defined in next section) ensures the achievement of steady state. All dynamical quantities are calculated in the steady state for a fixed set of values of the temperature ( $T$ ) and amplitude ( $h_0$ ) of the oscillating magnetic field. Then the temperature is reduced (by a small step) keeping the values of other parameters unchanged and a similar process (described above) is repeated. Here, the last spin configuration is used as the initial state for the present

value of temperature. In this way the temperature variations of all dynamical quantities are studied. Here, the temperature and field amplitudes are measured in the unit where,  $K_B = 1$  and  $J_F = 1$ .

### III. Numerical results:

The zero temperature configuration of this system is all spins are parallel in all layers and the adjacent layers contains antiparallel spins. The system can be decomposed in two different sublattices (say A and B). So, alternate layers form a sublattice. In a particular sublattice (A), the instantaneous magnetization is  $M_A(t) = 2(\sum_i s_i)/L^3$ . The time average (over a full cycle of the oscillating magnetic field) magnetization (for sublattice A) is  $Q_A = \frac{\omega}{2\pi} \oint M_A(t) dt$ . In the present study the frequency of the oscillating magnetic field is taken  $\omega = 2\pi f = 2\pi \times 0.01$ . The frequency ( $f$ ) of the oscillating magnetic field is kept constant ( $f = 0.01$ ) throughout the study. So, one complete oscillation would require 100 MCS. Initially, data for 1200 such cycles are discarded and average value of  $Q_A$  is calculated from next 300 cycles. It is checked that 300 number of cycles are sufficient to achieve the dynamically stable values of quantities. The dynamic order parameter  $Q_B$  for other sublattice (B) is calculated in the same way. The staggered dynamic order parameter  $Q_S$  is calculated as the time average (over a full cycle of the oscillating magnetic field) of instantaneous staggered magnetization ( $\frac{M_A - M_B}{2}$ ). Here,  $Q_S = \frac{\omega}{4\pi} \oint (M_A(t) - M_B(t)) dt$ . The dynamical average energy is also calculated as  $E = \frac{\omega}{2\pi} \oint H(t) dt$ . The dynamical specific heat ( $C$ ) is defined as  $C = \frac{dE}{dT}$  [12]. The temperature variations (with step  $\Delta T = 0.05$ ) of  $Q_A$ ,  $Q_B$ ,  $Q_S$ ,  $E$  and  $C$  are studied here, considering the amplitude ( $h_0$ ) and frequency ( $f$ ) of the time dependent magnetic field as parameters in each case.

Figure-1 shows the temperature variations of dynamic quantities for fixed values of  $J_F = 1.0$ ,  $J_A = -1.0$ ,  $f = 0.01$  and for two different values ( $h_0 = 2.5$  and  $h_0 = 3.0$ ). Figure-1(a) shows the temperature variations of the sublattice dynamic order parameters ( $Q_A$  and  $Q_B$ ). This variations clearly shows the two dynamic transitions near  $T_d = 2.2$  for  $h_0 = 2.5$  and  $T_d = 1.35$  for  $h_0 = 3.0$ . One can easily visualize the temperature variations (not shown) of dynamic staggered order parameters ( $Q_S$ ). These transitions becomes more pronounced from the plot of temperature variations of the derivatives ( $\frac{dQ_S}{dT}$ )

(in Figure-1(b)). The sharp minima (eventually divergences in  $L \rightarrow \infty$  limit) indicate the dynamic transition temperatures  $T_d = 2.20$  and  $T_d = 1.35$  for  $h_0 = 2.5$  and  $h_0 = 3.0$  respectively. These two dynamic transition were reconfirmed and re-estimated *independently* from the studies of the temperature variations of dynamic specific heat ( $C$ )[12]. It may be mentioned here that the temperature variation of the dynamic specific heat is not studied by previous meanfield calculations[10] These variations are shown in Figure-1(c). Here also, the dynamic specific heat ( $C$ ) shows peaks (eventually divergences in the limit  $L \rightarrow \infty$ ) near  $T_d = 2.20$  and  $T_d = 1.35$  for  $h_0 = 2.5$  and  $h_0 = 3.0$  respectively. In this way, the transition temperatures for the dynamic phase transitions are estimated over the range of values of the amplitudes of the oscillating magnetic field. Thus for fixed values of  $J_A = -1.0$ ,  $J_F = 1.0$  and  $f = 0.01$ , the dynamic phase boundary is obtained.

To study the variations of dynamic phase boundary with the relative strength of the antiferromagnetic interactions ( $J_A$ ), the similar investigations are made for  $J_A = -0.5$  and  $J_F = 1.0$ . In this case, the relative antiferromagnetic strength is reduced. Figure-2(a) shows the temperature variations of the derivative of staggered dynamic order parameters, i.e.,  $\frac{dQ_S}{dT}$ . Like the previous cases, the  $\frac{dQ_S}{dT}$ , shows sharp minima indicating the dynamic phase transitions near  $T_d = 1.20$  for  $h_0 = 2.0$  and near  $T_d = 0.45$  for  $h_0 = 3.0$ . The same transition temperatures were recalculated from the temperature variations of dynamic specific heat ( $C$ ). The dynamic specific heat  $C$  shows sharp maxima near the same transition points indicating the dynamic transitions. These results are shown in Figure-2(b). In this way, the entire dynamic phase boundary is obtained.

For a comparison, the dynamic transitions are studied for a pure ferromagnetic system. The transition temperatures  $T_d = 1.6$  and  $T_d = 0.8$  are obtained from the temperature variation of the derivative of dynamic order parameter  $\frac{dQ}{dT}$ , for  $Q = \frac{\omega}{2\pi} \oint M(t)dt$ , where  $M(t) = [M_A(t) + M_B(t)]$  is the total instantaneous magnetization obtained by putting  $J_F = 1.0$  and  $J_A = 1.0$  in equation (1). The dynamic transition temperatures are estimated from the sharp minima (shown in Figure-3) of  $\frac{dQ}{dT}$ . The results obtained here, are  $T_d = 1.6$  for  $h_0 = 2.0$  and  $T_d = 0.8$  for  $h_0 = 3.0$ . Hence the data for entire dynamic phase boundary are obtained.

The comprehensive results of the dynamic phase transitions are shown as the dynamic phase boundary in Figure-4. From the phase diagrams it is

clear that the shapes of dynamic phase boundaries for metamagnetic dynamic phase transitions are distinctly different from that for pure ferromagnets. Additionally, the dynamic phase boundary shrinks inward as the relative strength of antiferromagnetic interaction decreases. These phase diagrams for metamagnetic dynamic phase transitions agrees qualitatively well with those obtained from meanfield calculations[10].

#### IV. Concluding remarks:

The dynamic phase transition in Ising metamagnet driven by oscillating magnetic field is studied by Monte Carlo simulation. As far as the author's knowledge is concerned, this is the first Monte Carlo study of dynamic phase transition for this type of metamagnetic model. This study differs from the previous meanfield study[10] in the following aspects: *Firstly*, the dynamic phase transition was reconfirmed here from the temperature variation of dynamic specific heat[12], which was not done in meanfield study[10]. *Secondly*, in meanfield study, the multicritical behaviours are observed and the tricritical point was located on the phase boundary at lower temperatures. Here, in the Monte Carlo study, the probability of spin flip was calculated from the Gibb's distribution which provides good results in high temperature region. In the low temperature, region the quantum fluctuation will be excited and Quantum Monte Carlo will be the better method of study. For this reason, the phase boundary for very low temperature is not drawn.

In the present study, the order of transition is not mentioned. As a result one cannot be able to guess about the multicritical behaviour. Here, only the dynamic *transition* is observed. It may be mentioned here, that the existence of tricritical point was found[13] on the dynamic phase boundary by Monte Carlo simulation in pure Ising ferromagnet. However, this was disproved[14] later from the Monte Carlo study with larger lattice size and improved statistics. So, it is better not to mention about multicritical behaviour from the present Monte Carlo study of such small system size ( $L = 20$ ).

The shapes of the dynamic phase boundary depend on the relative antiferromagnetic strength as well the the frequencies of the oscillating magnetic field. In the present case, this variation with frequency is not studied. It may be an interesting study.

Above all, this dynamic phase transition in Ising metamagnets gives interesting result, theoretically. The physical reason of the dynamic phase

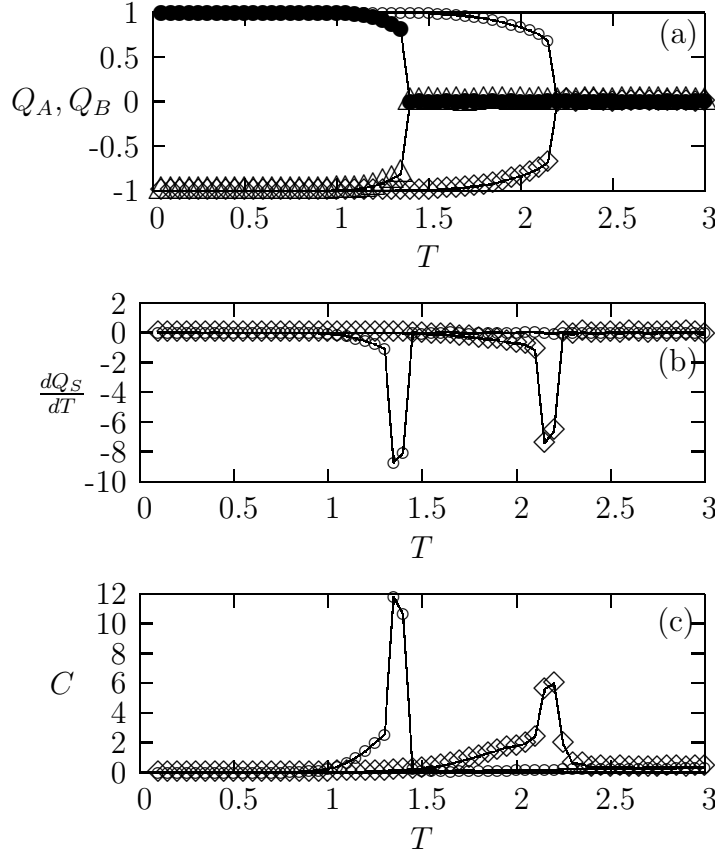
transition in metamagnet may be stated qualitatively as follows: for small values of the amplitude of the field and at low temperature, the instantaneous staggered magnetization oscillates about a nonzero value, giving rise to ordered phase. However, for large value of field amplitude and at high temperature, the instantaneous staggered magnetization oscillates symmetrically about a value very close to zero, leading to disordered phase. One has to see the hysteretic loop ( $m - h$ ) [1] to get the clear idea about the physical interpretation of the dynamic phase transition. The asymmetric  $m - h$  loop gives the dynamically ordered phase and the symmetric  $m - h$  loop gives disordered phase. In the case of metamagnet, this  $m$  should be the staggered magnetization. This theoretical investigation is an appeal to the experimentalists to study the dynamic phase transition in anisotropic metamagnet, like  $\text{FeBr}_2$ . Experimentally the existence of dynamic transition was found [7, 8] in Co film (ferromagnetic) on Cu surface (at room temperature) by surface magneto optic Kerr effect. Let us hope that the experimental study of dynamic phase transition in metamagnetic systems like  $\text{FeBr}_2$  driven by oscillating magnetic field, will bring some new physics in future.

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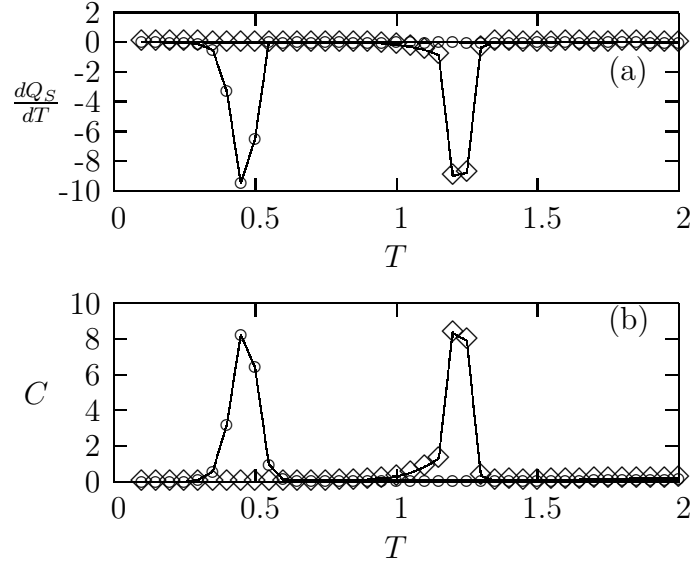
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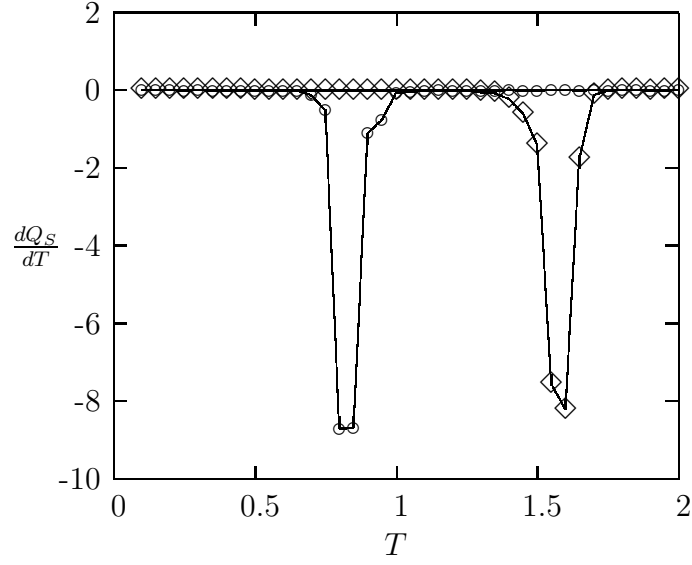




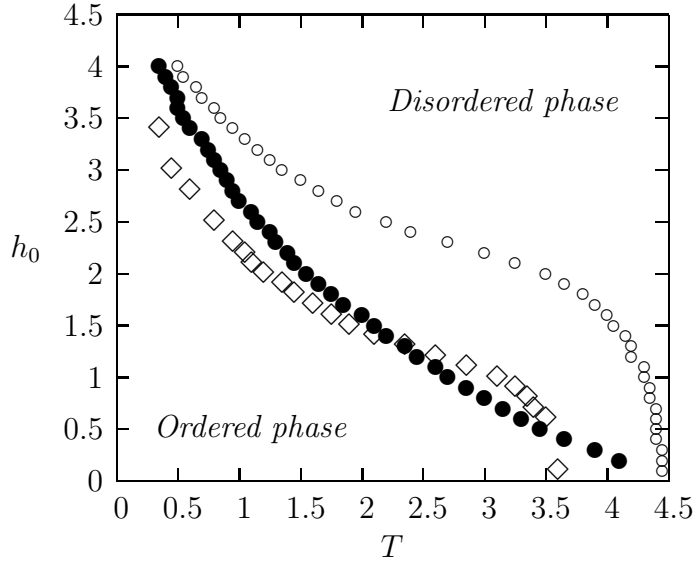
**Fig-1.** The temperature variations of (a) sublattice dynamic order parameters  $Q_A$  ( $\bullet$ ) for  $h_0 = 3.0$  and ( $\circ$ ) for  $h_0 = 2.5$ ) and  $Q_B$  ( $\triangle$  for  $h_0 = 3.0$  and ( $\diamond$ ) for  $h_0 = 2.5$ ), (b) the derivative ( $\frac{dQ_S}{dT}$ ) of staggered dynamic order parameter ( $Q_S$ ) ( $\circ$ ) for  $h_0 = 3.0$  and ( $\diamond$ ) for  $h_0 = 2.5$ ) and (c) the dynamic specific heat ( $C$ ) ( $\circ$ ) for  $h_0 = 3.0$  and ( $\diamond$ ) for  $h_0 = 2.5$ ). The continuous lines in all cases joining the data points act as guides to the eye. Here,  $J_A = -1 \times J_F$ . The  $T_d(h_0 = 2.5) = 2.2$  and  $T_d(h_0 = 3.0) = 1.35$ .



**Fig-2.** The temperature variations of (a)  $\frac{dQ_S}{dT}$  for  $h_0 = 3.0$  (o) and  $h_0 = 2.0$  ( $\diamond$ ) and (b)  $C$  for  $h_0 = 3.0$  (o) and  $h_0 = 2.0$  ( $\diamond$ ). The continuous lines in all cases joining the data points act as guides to the eye. Here,  $J_A = -0.5J_F$ .  $T_d(h_0 = 3.0) = 0.45$  and  $T_d(h_0 = 2.0) = 1.20$ .



**Fig-3.** The temperature variations of  $\frac{dQ_S}{dT}$  for  $h_0 = 2.0(T_d = 1.6)(\diamond)$  and  $h_0 = 3.0(T_d = 0.8)(o)$  for pure ferromagnetic ( $J_F = J_A = 1.0$ ) case.



**Fig-4.** The phase diagram of dynamic phase transitions. Metamagnetic dynamic phase boundaries (i) (◊) for  $J_A = -0.5$  and  $J_F = 1.0$  and (ii) (o) for  $J_A = -1.0$  and  $J_F = 1.0$ . The (•) represents the dynamic phase boundary of pure Ising ferromagnets ( $J_A = J_F = 1.0$ ).